arXiv:0910.3241v1 [math.NA] 16 Oct 2009

Interpolation and Iteration for Nonlinear Filters

Alexandre J. Chorin and Xuemin Tu

Department of Mathematics,
University of California at Berkeley and Lawrence Berkeley National Laboratory,
Berkeley, CA, 94720

Abstract

We present a general form of the iteration and interpolation process used in implicit particle filters. Implicit filters are based on a pseudo-Gaussian representation of posterior densities, and are designed to focus the particle paths so as to reduce the number of particles needed in nonlinear data assimilation. Examples are given.

Keywords: Implicit sampling, filter, pseudo-Gaussian, Jacobian, chainless sampling, particles

1 Introduction

There are many problems in science in which the state of a system must be identified from an uncertain equation supplemented by a stream of noisy data (see e.g. [7]). A natural model of this situation consists of an Ito stochastic differential equation (SDE):

$$dx = f(x,t)\,dt + g(x,t)\,dw, \tag{1}$$

where $x = (x_1, x_2, \ldots, x_m)$ is an m-dimensional vector, w is m-dimensional Brownian motion, f is an m-dimensional vector function, and $g(x,t)$ is an m by m diagonal matrix. The initial state x^0 is assumed given and may be random as well.

As the solution of the SDE unfolds, it is observed, and the values b^n of a measurement process are recorded at times $t^n, n = 1, 2, ...$ For simplicity assume $t^n = n\delta$, where δ is a fixed time interval. The measurements are related to the evolving state $x(t)$ by

$$b^n = h(x^n) + QW^n, \tag{2}$$

where h is a k-dimensional, generally nonlinear, vector function with $k \leq m$, Q is a k by k diagonal matrix, $x^n = x(n\delta)$, and W^n is a vector whose components are k independent Gaussian variables of mean zero and variance one, independent also of the Brownian motion in equation (1). The task is to estimate x on the basis of equation (1) and the observations (2).

If the system (1) and equation (2) are linear and the data are Gaussian, the solution can be found via the Kalman-Bucy filter (see e.g. [3]). In the general case, it is natural to try to estimate x via its evolving probability density. The initial state x^0 is known and so is its probability density; all one has to do is evaluate sequentially the density P_{n+1} of x^{n+1} given the probability densities P_k of x^k for $k \leq n$ and the data b^{n+1}. This can be done by following "particles" (replicas of the system) whose empirical distribution approximates P_n. A standard construction (see e.g [13, 12, 8, 1, 11, 5, 10, 9])

uses the probability density function (pdf) P_n and equation (1) to generate a prior density, and then uses the new data b^{n+1} to generate a posterior density P_{n+1} through weighting and resampling. In addition, one has to sample backward to take into account the information each measurement provides about the past, as well as avoid having too many identical particles after resampling. This can be very expensive, in particular because the number of particles needed can grow catastrophically (see e.g. [14, 2] and also Example 2 below). Sophisticated methods for generating efficient priors can be found e.g. in [8, 1]. The challenge is to generate high probability samples so as to minimize the effort of computing particle paths whose weight is very low.

In [6] we introduced an alternative to the standard approach. In our method the posterior density is sampled directly by iteration and interpolation, as suggested by our earlier work on chainless sampling [4], and by the observation in [15] connecting interpolation and the marginalization process used in chainless sampling. The new filter aims the particle trajectories as accurately as possible in the direction of the observations so that fewer particles are needed. In that earlier paper our approach was presented by means of simple examples. In the present paper we present a general, more abstract, formulation, introduce an extension to the case of sparse observations, and discuss additional examples.

2 Forward step

To begin, assume that at time $t^n = n\delta$, where $\delta > 0$ is fixed, we have a collection of M particles X_i^n, $1 \le i \le M$, $n = 0, 1, \ldots$, whose empirical density approximates P_n, the probability density at time $n\delta$ of the particles that obey the evolution equation (1) subject to the observations (2) at times $t = k\delta$ for $k \le n$. In the present section we explain how to find positions for the same particles at time $(n+1)\delta$ given only the positions at time $n\delta$ and the pdf P_n, taking into account the next observation and the equation of motion. Let $N(a, v)$ denote a Gaussian variable of mean a and variance v. First, approximate the SDE (1) by a difference scheme of the form

$$X^{n+1} = X^n + F(X^n, t^n)\delta + G(X^n, t^n)V^{n+1}, \tag{3}$$

where we assume temporarily that δ equals the interval between observations, i.e., we assume that there is an observation at every time step. X^n stands for $X(n\delta)$, G is assumed to be diagonal, and X^n, X^{n+1} are m dimensional vectors. F, G determine the scheme used to solve the SDE, see for example [6]. V^{n+1} is a vector of $N(0, \delta)$ Gaussian variables, independent of each other for each n, with the vectors V^{n+1} independent of each other for differing n, independent also of the W^k, $k = 1, ...$, in the observation equation (2). The sequence of $X^n, n = 0, 1, \ldots$ approximates a sample solution of the SDE, X^0 is assumed given and may be random. The function G in (3) does not depend on X^{n+1} for an Ito equation, and we assume for simplicity that F does not depend on X^{n+1} either, because this was the case in all the examples we have worked on so far. The analysis below can be easily repeated for the case where F does depend on X^{n+1}, at the cost of slightly more complicated formulas. Equation (3) states that $X^{n+1} - X^n$ is an $N(F(X^n, t^n)\delta, \delta G(X^n, t^n)^* G(X^n, t^n))$ vector, where the star * denotes a transpose.

We have one sample solution X_i^n of the SDE for each particle. Our task is to sample, for each particle, the vector X_i^{n+1} whose probability density is determined by the approximation of the SDE as well as by the next observation for each of the M particles. We keep the notation X_i^{n+1} for the positions of the particles even though once the observation is taken into account these positions no longer coincide with the positions of sample solutions of equation (3).

Consider the i-th particle. We are going to work particle by particle, so that the particle index i will be temporarily suppressed. Suppose we already know the posterior vector X^{n+1}. Its probability

density P_{n+1} of X^{n+1} given X^n is

$$\begin{aligned} P_{n+1}(X^{n+1}) &= Z^{-1}\exp\Big(-\left(X^{n+1}-X^n-F_n\right)^*\left(G_n^*G_n\right)^{-1}\left(X^{n+1}-X^n-F_n\right)/2 \\ &\quad -\left(h(X^{n+1})-b^{n+1}\right)^*\left(Q^*Q\right)^{-1}\left(h(X^{n+1})-b^{n+1}\right)/2\Big), \end{aligned} \tag{4}$$

where the functions $F_n = F(X^n, t^n)\delta$, and $G_n = \sqrt{\delta}G(X^n, t^n)$ can be read from the approximation of the SDE, and Z is a normalization constant, the integral of the numerator over all X^{n+1} with X^n fixed. The value of this Z is not available. Our goal is to find samples X^{n+1} whose probability is high, and which are well distributed with respect to P_{n+1}. We do that by picking the probability in advance: we first pick samples of m $N(0,1)$ variables $(\xi_1, \xi_2, \ldots, \xi_m) = \xi$, whose joint pdf (probability density function) is $\exp(-\xi^*\xi/2))/(2\pi)^{m/2}$, and require that each X^{n+1} be a function of a sample ξ with the same probability as ξ, up to the Jacobian of the transformation. This should produce likely and well-distributed samples.

A little thought shows that this can be done, not by equating P_{n+1} to $\exp(-\xi^*\xi/2)/(2\pi)^{m/2}$, but by equating the arguments of the two exponentials. For example, if one wants to represent a $N(0,v)$ random variable x with pdf $\exp(-\frac{x^2}{2v})/\sqrt{2\pi v}$ as a function of a $N(0,1)$ variable ξ with pdf $\exp(-\xi^2/2)/\sqrt{2\pi}$, equating the arguments yields $x = \sqrt{v}\,\xi$, clearly a good choice. Thus, we wish to solve the equation

$$\begin{aligned} &\xi^*\xi/2 = \\ &= \left(X^{n+1}-X^n-F_n\right)^*\left(G_n^*G_n\right)^{-1}\left(X^{n+1}-X^n-F_n\right)/2 + \left(h(X^{n+1})-b^{n+1}\right)^*\left(Q^*Q\right)^{-1}\left(h(X^{n+1})-b^{n+1}\right)/2 \end{aligned} \tag{5}$$

and obtain X^{n+1} as a function of ξ.

We proceed point by point— given a vector ξ, we find the corresponding X^{n+1} rather than look for an expression for the function $X^{n+1}(\xi)$ as a whole—and by iteration: we find a sequence of approximations X_j^{n+1} ($= X_j$ for brevity) which converges to X^{n+1}; we set $X_0 = 0$, and now explain how to find X_{j+1} given X_j. First, expand the function h in the observation equation (2) in Taylor series around X_j:

$$h(X_{j+1}) = h(X_j) + H_j \cdot (X_{j+1} - X_j), \tag{6}$$

where H_j is a Jacobian matrix evaluated at X_j. The observation equation (2) can be approximated as:

$$z_j = H_j X_{j+1} + QW^{n+1}, \tag{7}$$

where $z_j = b^{n+1} - h(X_j) + H_j X_j$.

The left side of equation (5) can be approximated as:

$$\begin{aligned} &\left(X_{j+1}-X^n-F_n\right)^*\left(G_n^*G_n\right)^{-1}\left(X_{j+1}-X^n-F_n\right)/2 + \left(H_jX_{j+1}-z_j\right)^*\left(Q^*Q\right)^{-1}\left(H_jX_{j+1}-z_j\right)/2 \\ &= \left(X_{j+1}-\bar{m}_j\right)^*\Sigma_j^{-1}\left(X_{j+1}-\bar{m}_j\right)/2 + \Phi_j, \end{aligned} \tag{8}$$

where

$$\Sigma_j^{-1} = \left(G_n^*G_n\right)^{-1} + H_j^*(Q^*Q)^{-1}H_j, \quad \bar{m}_j = \Sigma_j\left(\left(G_n^*G_n\right)^{-1}(X^n+F_n) + H_j^*(Q^*Q)^{-1}z_j\right),$$

and

$$K_j = H_jG_n^*G_nH_j^* + Q^*Q, \quad \Phi_j = \left(z_j - H_j(X^n+F_n)\right)^*K_j^{-1}\left(z_j - H_j(X^n+F_n)\right)/2.$$

We now solve for X_{j+1} as a function of ξ. To make the computation tractable, in this step we ignore the remainder Φ_j; this is a key step. We thus solve the simpler equation

$$(X_{j+1} - \bar{m}_j)^* \Sigma_j^{-1} (X_{j+1} - \bar{m}_j)/2 = \xi^* \xi/2. \tag{9}$$

This can be done in any of a number of ways; for example, one can write $\Sigma_j = L_j L_j^*$, where L_j is a lower triangular matrix and L_j^* is its transpose, and then set $X_{j+1} = \bar{m}_j + L_j \xi$ (a different algorithm was suggested in [6]). The iteration is done.

If the sequence X_j converges to a limit, call the limit X^{n+1}. One can readily check that the approximate equation (7) converges to the full observation equation (2). The remainders Φ_j also converge to a limit Φ^{n+1}. Equation (5) becomes:

$$\begin{aligned} &\xi^* \xi/2 + \Phi^{n+1} = \\ &= \left(X^{n+1} - X^n - F_n\right)^* (G_n^* G_n)^{-1} \left(X^{n+1} - X^n - F_n\right)/2 + (h(X^{n+1}) - b^{n+1})(Q^*Q)^{-1}(h(X^{n+1}) - b^{n+1})/2. \end{aligned} \tag{10}$$

Multiply this equation by -1 and exponentiate both sides:

$$\begin{aligned} &\exp(-\xi^* \xi/2) \exp(-\Phi^{n+1}) = \\ &= \exp\left(- \left(X^{n+1} - X^n - F_n\right)^* (G_n^* G_n)^{-1} \left(X^{n+1} - X^n - F_n\right)/2 - \left(h(X^{n+1}) - b^{n+1}\right)^* (Q^*Q)^{-1} \left(h(X^{n+1}) - b^{n+1}\right)/2 \right). \end{aligned} \tag{11}$$

This differs from what we set out to do in equation (5) by the factor $\exp(-\Phi^{n+1})$ on the right hand side.

Let $P(\alpha|\beta)$ be the probability of α given β. The factor $\exp(-\Phi^{n+1})$ is proportional to $P(b^{n+1}|X^n)$, and equation (11) is the statement

$$P(X^{n+1}|X^n, b^{n+1}) P(b^{n+1}|X^n) = P(X^{n+1}|X^n) P(b^{n+1}|X^{n+1}), \tag{12}$$

i.e., this is Bayes' theorem. Note also that equation (9) is a pseudo-Gaussian representation of X^{n+1}, not a Gaussian representation; the matrix Σ_j is a function of the sample.

We next compute the Jacobian determinant $J = \det(\partial X^{n+1}/\partial \xi)$. This can be often done analytically. Equation (9) relates X^{n+1} to ξ implicitly. We have values of ξ and the corresponding values of X^{n+1}; to find J there is no need to solve again for X^{n+1}; an implicit differentiation is all that is needed. Alternately, J can be found numerically, by taking nearby values of ξ, redoing the iteration (which should converge in one step, because one can start from the known value of X^{n+1}), and differencing.

The expression on the right-hand side of equation (11) is proportional to $P(b^{n+1}|X^{n+1}) P(X^{n+1}|X^n)$, with a proportionality constant independent of X^n. When X^{n+1} is sampled as just described, each value of $X^{n+1} = X^{n+1}(\xi)$ appears with probability $\frac{1}{(2\pi)^{m/2}} \exp(-\xi^* \xi/2)/|J|$, and then the value of this expression is $\exp(-\xi^* \xi/2) \exp(-\Phi^{n+1})$. To get the right value of the expression on the average, one has to give each proposed X^{n+1} the sampling weight $W = \frac{1}{(2\pi)^{m/2}} \exp(-\Phi^{n+1})|J|$, (with another factor $P(X^n)$ if such factors are not all equal). Since $\frac{1}{(2\pi)^{m/2}}$ is a constant and the same to every particle, we will drop it from now on. Here we see an advantage of starting from a prechosen reference variable ξ: the factor $\exp(-\xi^* \xi/2)$, which varies from sample to sample, has been discounted in advance and does not contribute to the non-uniformity of the weights. We shall see that the other factors can be expected to vary little.

Do this for all the particles and obtain new positions with weights $W_i = \exp(-\Phi_i^{n+1})|J_i|$, where Φ_i^{n+1}, J_i are the values of these quantities for the i-th particle. One can get rid of the weights after the fact by resampling, i.e., for each of M random numbers $\theta_k, k = 1, \ldots, M$ drawn from the uniform distribution on $[0, 1]$, choose a new $\widehat{X}_k^{n+1} = X_i^{n+1}$ such that $A^{-1}\sum_{j=1}^{i-1} W_j < \theta_k \leq A^{-1}\sum_{j=1}^{i} W_j$ (where $A = \sum_{j=1}^{M} W_j$), and then suppress the hat.

Note also that the resampling does not have to be done at every step- for example, one can add up the phases for a given particle and resample only when the ratio of the largest cumulative weight $\exp(-\sum(\phi_i - \log|J_i|))$ to the smallest such weight exceeds some limit L (the summation is over the weights accrued to a particular particle i since the last resampling). If one is worried by too many particles being close to each other ("depletion" in the usual Bayesian terminology), one can divide the set of particles into subsets of small size and resample only inside those subsets, creating a greater diversity. As will be seen in the numerical results section, none of these strategies is used here and we resample fully at every step.

The computational complexity of this construction depends on the sparseness of the matrix Σ_j, which depends on the sparseness of H_j in the expression (8), which depends on the structure of the function h in equation (2). In the frequently encountered situation where h is diagonal, in the sense that each quantity measured is a function of a single component of the vector whose dynamics are given by equation (1), one finds that Σ_j and H_j are diagonal, and the computations, including the computation of the Jacobian J, are easy, whether h is linear or not. The more arguments in each of the components of the function h, the more labor is required.

If both equations (1) and (2) are linear and the initial data are Gaussian, then the pdfs P_n are Gaussian. We only need to find the mean and the variance of the pdf, which can be found as above by considering a single particle; the iterations converge in one step. The resulting means and variances are identical to those produced by the Kalman filter. If one had needed multiple particles, their weights would have been all equal. If equation (1) is nonlinear but equation (2) is linear (or can be well approximated by a linear function in each interval $(n\delta, (n+1)\delta)$), then the P_{n+1} are in general not Gaussian and one needs multiple particles. The iterations still converge in one step, and what one obtains is a version of the forward step in a filter with an optimal importance function (as described e.g in [6]).

The convergence of the iteration will be very briefly discussed further below. We have chosen the variables ξ to be independent $N(0, 1)$ variables, but there is nothing sacred about this choice. The goal is to pick samples whose probability is high, and in some contexts other choices may be better. We will discuss those other choices when they are made in further work.

3 Backward sampling

In the previous section we described how to sample the pdf at time $(n + 1)\delta$ given the pdf at time $n\delta$. In general, this is not sufficient. Every observation provides information not only about the future but also about the past- it may, for example, tag as improbable earlier states that had seemed probable before the observation was made. Furthermore, in non-Gaussian settings, the pdf one obtains by going directly from time $(n - 1)\delta$ to step $(n + 1)\delta$ by a step of duration 2δ may be different from the pdf one obtains after two steps that include an intermediate step. After one has sampled at time $(n+1)\delta$, one has to go back, correct the past, and resample (this backward sampling is often misleadingly explained in the literature solely by the need to create greater diversity among the particles). We resample by interpolation, which we present explicitly for one backward step. It is quite obvious one can do that for as many backward steps as are needed.

Given a set of particles at time $(n+1)\delta$, after a forward step and maybe a subsequent resampling,

one can figure out where each particle i was in the previous two steps, and have a partial history for each particle i: $X_i^{n-1}, X_i^n, X_i^{n+1}$ (if resamplings had occurred, some parts of that history may be shared among several current particles). Knowing the first and the last members of this sequence, we recompute X^n by interpolation, thus projecting information backward one step.

The probability of the $X^{\rm new}$ that will replace X^n is the product of the three probabilities (properly normalized): the probability of the new leg from X^{n-1} to X^n, the probability of the resulting leg from X^n to X^{n+1} (the end result being known), and the probability of the resulting observation at time $n\delta$, i.e.:

$$\exp\Big(-\left(X^{\rm new}-X^{n-1}-F_{n-1}\right)^*(G_{n-1}^*G_{n-1})^{-1}\left(X^{\rm new}-X^{n-1}-F_{n-1}\right)/2$$
$$-\left(X^{n+1}-X^{\rm new}-F_n\right)^*(G_n^*G_n)^{-1}\left(X^{n+1}-X^n-F_n\right)/2-(h(X^{\rm new})-b^n)^*(Q^*Q)^{-1}(h(X^{\rm new})-b^n)/2\Big). \tag{13}$$

Here we recall that $F_{n-1}=F(X^{n-1},t^{n-1})\delta$ and $G_{n-1}=\sqrt{\delta}G(X^{n-1},t^{n-1})$ are known from the approximation of the SDE, F_n and G_n are functions of $X^{\rm new}$, and the subscript i referring to the particle has been omitted. This expression differs from equation (4) by having an additional exponential factor.

Once again, we set up an iteration, with iterates X_j, that converges to $X^{\rm new}$, and start with $X_0=0$. We expand $h(X_{j+1})$ in a Taylor series around X_j, so that the last factor in the expression (13) becomes a quadratic in X_{j+1}. We complete squares so that the argument of the exponential in (13) can be written as $(X_{j+1}-\bar m_j)\Sigma_j^{-1}((X_{j+1}-\bar m_j)/2+\Phi_j$; equate $(X_{j+1}-\bar m_j)\Sigma_j^{-1}((X_{j+1}-\bar m_j)/2$ to $\xi^*\xi/2$, solve to get X_{j+1} as a function of ξ, calculate the Jacobian, and find the weight. We do this for all the particles, and resample as needed. This concludes the backward sampling step. Note that as a result of the backward step and the subsequent forward step, P_{n+1} depends, not only on the positions of the particles at time $n\delta$, but also on the earlier history of the system.

4 Sparse observations

Consider now a situation where we do not have observations at every time step. First, assume that one has observation at time $(n+1)\delta$ but not at time $n\delta$. We try to sample X^n and X^{n+1} together given the observation information at time step $(n+1)\delta$. Consider the i-th particle. Suppose we are given the vector X_i^{n-1} for that particle. Suppress again the particle index i. The joint probability density $P_{n,n+1}$ of X^n and X^{n+1} given X^{n-1} is

$$P_{n,n+1}(X^n,X^{n+1})$$
$$=Z^{-1}\exp\Big(-\left(X^n-X^{n-1}-F_{n-1}\right)^*(G_{n-1}^*G_{n-1})^{-1}\left(X^n-X^{n-1}-F_{n-1}\right)/2$$
$$-\left(X^{n+1}-X^n-F_n\right)^*(G_n^*G_n)^{-1}\left(X^{n+1}-X^n-F_n\right)/2-\left(h(X^{n+1})-b^{n+1}\right)^*(Q^*Q)^{-1}\left(h(X^{n+1})-b^{n+1}\right)/2\Big), \tag{14}$$

where Z is the normalization constant. We recall that $F_{n-1}=F(X^{n-1},t^{n-1})\delta$, $G_{n-1}=\sqrt{\delta}G(X^{n-1},t^{n-1})$ are known from the approximation of the SDE, F_n and G_n depend on X^n.

In the now familiar sequence of steps, we pick two independent samples ξ_n and ξ_{n+1}, each with

probability density $\exp(-\xi^*\xi/2)/(2\pi)^{m/2}$, and try to solve the equation

$$\begin{aligned}
&{\xi_n}^*\xi_n/2 + \xi_{n+1}^*\xi_{n+1}/2 \\
&= \left(X^n - X^{n-1} - F_{n-1}\right)^* (G_{n-1}^* G_{n-1})^{-1} \left(X^n - X^{n-1} - F_{n-1}\right)/2 \\
&\quad + \left(X^{n+1} - X^n - F_n\right)^* (G_n^* G_n)^{-1} \left(X^{n+1} - X^n - F_n\right)/2 + \left(h(X^{n+1}) - b^{n+1}\right)^* (Q^*Q)^{-1} \left(h(X^{n+1}) - b^{n+1}\right)/2,
\end{aligned} \tag{15}$$

to obtain X^n and X^{n+1} as functions of ξ_n and ξ_{n+1}.

We define a sequence of approximations X_j^n and X_j^{n+1} which converge to X^n and X^{n+1}, respectively; set $X_0^n = 0$ and $X_0^{n+1} = 0$, and at each iteration find X_{j+1}^n and X_{j+1}^{n+1} given X_j^n and X_j^{n+1}. First, expand the function h in the observation equation (2) in Taylor series around X_j^{n+1}:

$$h(X_{j+1}^{n+1}) = h(X_j^{n+1}) + H_j^{n+1} \cdot (X_{j+1}^{n+1} - X_j^{n+1}), \tag{16}$$

where H_j^{n+1} is a Jacobian matrix evaluated at X_j^{n+1}. The observation equation (2) is approximated as:

$$z_j^{n+1} = H_j^{n+1} X_{j+1}^{n+1} + QW^{n+1}, \tag{17}$$

where $z_j^{n+1} = b^{n+1} - h(X_j^{n+1}) + H_j^{n+1} X_j^{n+1}$.

Let $F_{n,j} = F(X_j^n, t^n)\delta$ and $G_{n,j} = \sqrt{\delta} G(X_j^n, t^n)$. The right side of equation (15) can be approximated as:

$$\begin{aligned}
&\left(X_{j+1}^n - X^{n-1} - F_{n-1}\right)^* (G_{n-1}^* G_{n-1})^{-1} \left(X_{j+1}^n - X^{n-1} - F_{n-1}\right)/2 \\
&+ \left(X_{j+1}^{n+1} - X_{j+1}^n - F_{n,j}\right)^* (G_{n,j}^* G_{n,j})^{-1} \left(X_{j+1}^{n+1} - X_{j+1}^n - F_{n,j}\right)/2 \\
&+ \left(H_j^{n+1} X_{j+1}^{n+1} - z_j^{n+1}\right)^* (Q^*Q)^{-1} \left(H_j^{n+1} X_{j+1}^{n+1} - z_j^{n+1}\right)/2.
\end{aligned} \tag{18}$$

We first combine the last two terms in (18) and obtain

$$\begin{aligned}
&\left(X_{j+1}^{n+1} - X_{j+1}^n - F_{n,j}\right)^* (G_{n,j}^* G_{n,j})^{-1} \left(X_{j+1}^{n+1} - X_{j+1}^n - F_{n,j}\right)/2 + \left(H_{n+1} X_{j+1}^{n+1} - z^{n+1}\right)^* (Q^*Q)^{-1} \left(H_{n+1} X_{j+1}^{n+1} - z^{n+1}\right)/2 \\
&= \left(X_{j+1}^{n+1} - \bar{m}_j^{n+1}\right)^* (\Sigma_j^{n+1})^{-1} \left(X_{j+1}^{n+1} - \bar{m}_j^{n+1}\right)/2 + \Phi_j^{n+1},
\end{aligned} \tag{19}$$

where

$$\begin{aligned}
(\Sigma_j^{n+1})^{-1} &= (G_{n,j}^* G_{n,j})^{-1} + (H_j^{n+1})^* (Q^*Q)^{-1} H_j^{n+1}, \\
\bar{m}_j^{n+1} &= \Sigma_j^{n+1} \left((G_{n,j}^* G_{n,j})^{-1} (X_{j+1}^n + F_{n,j}) + (H_j^{n+1})^* (Q^*Q)^{-1} z_j^{n+1} \right), \\
K_j^{n+1} &= H_j^{n+1} G_{n,j}^* G_{n,j} (H_j^{n+1})^* + Q^*Q,
\end{aligned}$$

and

$$\Phi_j^{n+1} = \left(z_j^{n+1} - H_j^{n+1}(X_{j+1}^n + F_{n,j})\right)^* (K_j^{n+1})^{-1} \left(z_j^{n+1} - H_j^{n+1}(X_{j+1}^n + F_{n,j})\right)/2.$$

We combine the first term in (18) and the second term in (19) and obtain

$$\begin{aligned}
&\left(X_{j+1}^n - X^{n-1} - F_{n-1}\right)^* (G_{n-1}^* G_{n-1})^{-1} \left(X_{j+1}^n - X^{n-1} - F_{n-1}\right)/2 + \Phi_j^{n+1} \\
= \;& \left(X_{j+1}^n - X^{n-1} - F_{n-1}\right)^* (G_{n-1}^* G_{n-1})^{-1} \left(X_{j+1}^n - X^{n-1} - F_{n-1}\right)/2 \\
& + \left(z_j^{n+1} - H_j^{n+1}(X_{j+1}^n + F_{n,j})\right)^* (K_j^{n+1})^{-1} \left(z_j^{n+1} - H_j^{n+1}(X_{j+1}^n + F_{n,j})\right)/2 \\
= \;& \left(X_{j+1}^n - \bar{m}_j^n\right)^* (\Sigma_j^n)^{-1} \left(X_{j+1}^n - \bar{m}_j^n\right)/2 + \Phi_j^n,
\end{aligned} \tag{20}$$

where

$$(\Sigma_j^n)^{-1} = (G_{n-1}^* G_{n-1})^{-1} + (H_j^{n+1})^* (K_j j^{n+1})^{-1} H_j^{n+1},$$
$$\bar{m}_j^n = \Sigma_j^n \left((G_{n-1}^* G_{n-1})^{-1} (X^{n-1} + F_{n-1}) + (H_j^{n+1})^* (K_j^{n+1})^{-1} (z_j^{n+1} - H_j^{n+1} F_{n,j}) \right),$$
$$K_j^n = H_j^{n+1} G_{n-1}^* G_{n-1} (H_j^{n+1})^* + K_j^{n+1},$$

and

$$\Phi_j^n = \left(z_j^{n+1} - H_j^{n+1}(F_{n,j} + X^{n-1} + F_{n-1}) \right)^* (K_j^n)^{-1} \left(z_j^{n+1} - H_j^{n+1}(F_{n,j} + X^{n-1} + F_{n-1}) \right)/2.$$

Combining (15), (16), (18), (19), and (20), we try to solve

$$\begin{aligned} &{\xi_n}^* \xi_n/2 + \xi_{n+1}^* \xi_{n+1}/2 \\ &= \left(X_{j+1}^{n+1} - \bar{m}_j^{n+1} \right)^* (\Sigma_j^{n+1})^{-1} \left(X_{j+1}^{n+1} - \bar{m}_j^{n+1} \right)/2 + \left(X_{j+1}^n - \bar{m}_j^n \right)^* (\Sigma_j^n)^{-1} \left(X_{j+1}^n - \bar{m}_j^n \right)/2 + \Phi_j^n. \end{aligned} \tag{21}$$

We now solve for X_{j+1}^n and X_{j+1}^{n+1} as functions of ξ_n and ξ_{n+1}, ignoring the remainders Φ_j^n, i.e. we solve the simpler equations

$$(X_{j+1}^k - \bar{m}_j^k)^* (\Sigma_j^k)^{-1} (X_{j+1}^k - \bar{m}_j^k)/2 = \xi_k^* \xi_k/2, \quad k = n, n+1 \tag{22}$$

If the sequences X_j^n and X_j^{n+1} converge to limits, call the limits X^n and X^{n+1}. In the limit, the approximate equation (17) converges to the full observation equation (2). The remainders Φ_j^n and Φ_j^{n+1} also converge to limits Φ^n and Φ^{n+1}. Equation (15) becomes:

$$\begin{aligned} &\xi_n^* \xi_n/2 + \xi_{n+1}^* \xi_{n+1}/2 + \Phi^n \\ = \;& \left(X^n - X^{n-1} - F_{n-1} \right)^* (G_{n-1}^* G_{n-1})^{-1} \left(X^n - X^{n-1} - F_{n-1} \right)/2 \\ &+ \left(X^{n+1} - X^n - F_n \right)^* (G_n^* G_n)^{-1} \left(X^{n+1} - X^n - F_n \right)/2 + (h(X^{n+1}) - b^{n+1})(Q^* Q)^{-1} (h(X^{n+1}) - b^{n+1})/2. \end{aligned} \tag{23}$$

Multiply by -1 and exponentiate:

$$\begin{aligned} &\exp(-\xi_n^* \xi_n/2) \exp(-\xi_{n+1}^* \xi_{n+1}/2) \exp(-\Phi^n) \\ = \;& \exp\Big(\left(X^n - X^{n-1} - F_{n-1} \right)^* (G_{n-1}^* G_{n-1})^{-1} \left(X^n - X^{n-1} - F_{n-1} \right)/2 \\ + \;& \left(X^{n+1} - X^n - F_n \right)^* (G_n^* G_n)^{-1} \left(X^{n+1} - X^n - F_n \right)/2 + \left(h(X^{n+1}) - b^{n+1} \right)^* (Q^* Q)^{-1} (h(X^{n+1}) - b^{n+1}) \big)/2 \Big). \end{aligned} \tag{24}$$

As before, one has to give each proposed X^n and X^{n+1} the sampling weight $W = \exp(-\Phi^n)|J|$, where J is the Jacobian $J = \det(\partial(X^n, X^{n+1})/\partial(\xi_n, \xi_{n+1}))$ which must be computed. One does this for all particles and resamples as needed. This process can be generalized if one wishes to sample at more times between observations. One should also note that the procedure just described may make the evaluation of Jacobians significantly more onerous, but still often tractable.

The construction of this paragraph is important because many data sets one tries to assimilate are indeed sparse, and also for the following reason. We have not provided in this present paper a discussion of the convergence of the iterations we use. This convergence depends on the structure of the underlying SDE, on the scheme used to approximate it, and on the specific ways one solves for the new increments in terms of the reference variables ξ, and cannot be analyzed without considering these specifics. In our previous paper [6] we analyzed a special case and found that there the convergence depended on the size of the time step. We conjecture that this happens frequently. The present section provides a way to decrease the time step as a device for repairing diverging iterations without much additional thought.

5 Example 1

We apply our filter to a prototypical marine ecosystem model studied in [10]. We set the main parameters equal to the ones in [10]; however, we will also present some results with a range of noise variances to make a particular point. We did the data assimilation with the filter described above, without back sampling, and also by the a standard particle filter SIR (Sampling importance resampling), see [1].

The model involves four state variables: phytoplankton P (microscopic plants), zooplankton Z (microscopic animals), nutrients N (dissolved inorganics), and detritus D (particulate organic non-living matter). At the initial time $t = 0$ we have $P(0) = 0.125$, $Z(0) = 0.00708$, $N(0) = 0.764$, and $D(0) = 0.136$. The system is described by the following nonlinear ordinary differential equations, explained in [10]:

$$\begin{aligned}
\frac{dP}{dt} &= \frac{N}{0.2+N}\gamma P - 0.1P - 0.6\frac{P}{0.1+P}Z + N(0,\sigma_P^2) \\
\frac{dZ}{dt} &= 0.18\frac{P}{0.1+P}Z - 0.1Z + N(0,\sigma_Z^2) \\
\frac{dN}{dt} &= 0.1D + 0.24\frac{P}{0.1+P}Z - \gamma P\frac{N}{0.2+N} + 0.05Z + N(0,\sigma_N^2) \\
\frac{dD}{dt} &= -0.1D + 0.1P + 0.18\frac{P}{0.1+P}Z + 0.05Z + N(0,\sigma_D^2),
\end{aligned} \tag{25}$$

where the parameter γ, the " growth rate", is determined by the equations given by

$$\gamma_t = 0.14 + 3\Delta\gamma_t, \quad \Delta\gamma_t = 0.9\Delta\gamma_{t-1} + N(0,\sigma_\gamma^2).$$

The variances of the noise terms are: $\sigma_P^2 = (0.01P(0))^2$, $\sigma_Z^2 = (0.01Z(0))^2$, $\sigma_N^2 = (0.01N(0))^2$, $\sigma_D^2 = (0.01D(0))^2$, and $\sigma_\gamma^2 = (0.01)^2$.

The observations were obtained from NASA's SeaWiFS satellite ocean color images. These observations provide a time series for phytoplankton; the relation between the observations $P(t)_{\text{obs}}$ (corresponding to the vector b^n in the earlier discussion) and the solution $P(t)$ of the equation of the first equation in (25) is assumed to be:

$$\log P(t)_{\text{obs}} = \log P(t) + N(0,\sigma_{\text{obs}}^2),$$

where $\sigma_{\text{obs}}^2 = 0.3^2$. Note that this observation equation is not linear. There are 190 data points distributed from late 1997 to mid 2002. The sample intervals ranged from a week to a month or more, for details see [10]. As in [10], we discretize the system (25) by an Euler method with $\Delta t = 1$ day and prohibit the state variables from dropping below 1 percent of their initial values.

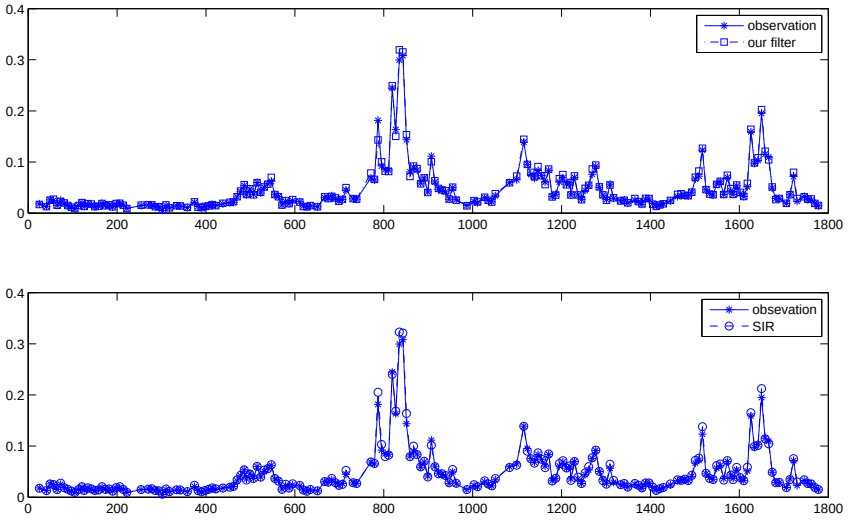
We have compared our filter and SIR in three sets of numerical experiments, all with the same initial values as listed above. In each case we attempted to find a trajectory of the system consistent with the fixed data, and observed how well we succeeded. In the first set of the experiments, we used 100 particles and take $\sigma_P^2 = (0.01P(0))^2$ as in [10]. In this case, the (assumed) variance of the system is much smaller than the (assumed) variance of the observations; the particle paths are bunched close together, and the results from our filter and from SIR are quite close, see Figure 1, where we plotted the P component of the reconstructed solution as well as the corresponding data.

In the second set of the experiments, we still used 100 particle but assumed $\sigma_p^2 = (P(0))^2$. The variance of the system is now comparable to the variance of the observation. For SIR, after resampling, the number of the distinct particles is smaller than in the first case, as a result of the loss

Table 1: The number of distinct particles after resampling with different system variances and different numbers of particles

σ_p	# particle	average # particles left after resampling	
		SIR	Our filter
$0.01P(0)$	100	61	61
$P(0)$	100	19	63
$P(0)$	10	2.2	6.3

Figure 1: Results with $\sigma_P^2 = (0.01P(0))^2$ and 100 particles



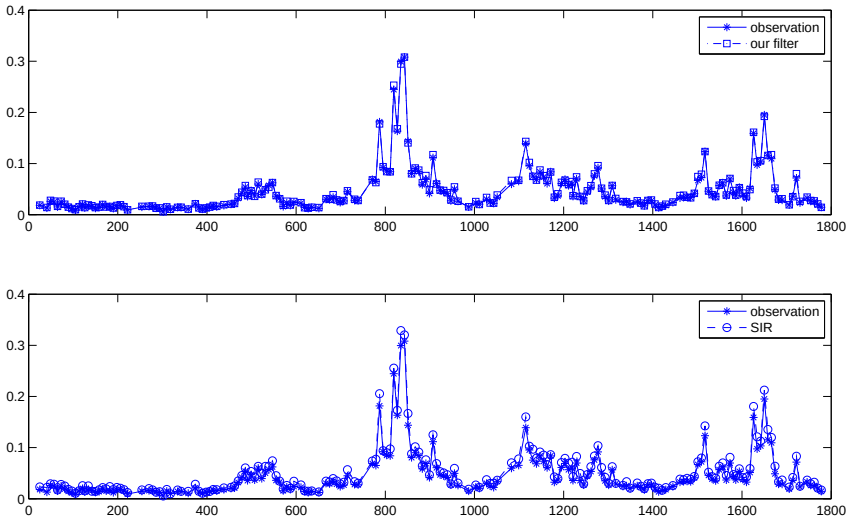
of diversity after resampling when the weights are very different from each other, see Table 1, where we exhibit the average number of distinct particles left after each resample; there is a resample after each step. Remember that there is some loss of diversity in resampling even if all the weights are equal. With 100 particles, the filtered results with SIR are still comparable to those with our filter. See Figure 2.

In the third set of the experiments, we used only 10 particles and kept $\sigma_p^2 = (P(0))^2$. As one could have foreseen, our filter does better than SIR, see Figure 3. One should remember however that we are working with a low dimensional problem where the differences between filters are not expected to be very significant; the cost if 100 particles is not prohibitive.

6 Example 2

We consider next a simple high dimensional example, used in [14] to show how particle filters fail when the number of dimensions is large. We assume that each component of X^n is an independent

Figure 2: Results with $\sigma_P^2 = P(0)^2$ and 100 particles



Gaussian with zero mean and unit variance. This is equivalent to taking $\delta = 1$, $F(X^n, \delta) = 0$, $G(X^n, t^n) = I$ in equation (3), and eliminating the X^n term. We have

$$X^n = V^n.$$

Each component of X^n is observed individually, so that

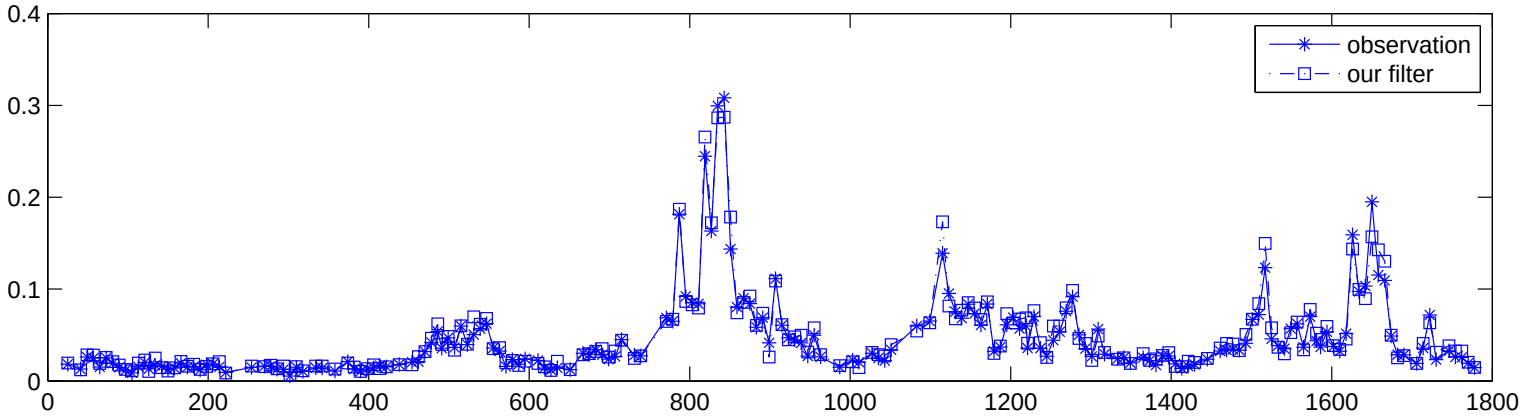
$$b^n = X^n + W^n.$$

We implement our filter with these particular choices. At the j-th iteration, $H_j = I$ in equation (6) and $z_j = b^{n+1}$ in equation (7). Therefore, we have $\Sigma_j^{-1} = 2I$, $\bar{m}_j = b^{n+1}/2$, and $\Phi_j = (b^{n+1})^* b^{n+1}/4$, in equation (8). The iterations converge in one step and all the particles have the same weights.

However, with SIR the weights are uneven. We ran the SIR filter 1000 times, with a 1000 particles each time; in each run we normalized the weights so that add up to one, and we recorded the maximum weight. In Figures 4 we display a histogram of these recorded maximum weights. As one can observe, when the number of dimensions is large, most of time, a single particle in each run hogs all the probability, and this version of SIR fails.

7 Conclusions

We have presented a general form of the iteration and interpolation process used in our new implicit nonlinear particle filter. The goal is to aim particle paths sharply so that fewer are needed. We conjecture that there is no general way to reduce the variability of the weights in particle sampling further than we have. We also presented additional simple examples that illustrate the potential of this new sampling. These examples are simple in that one is low-dimensional, while the second is



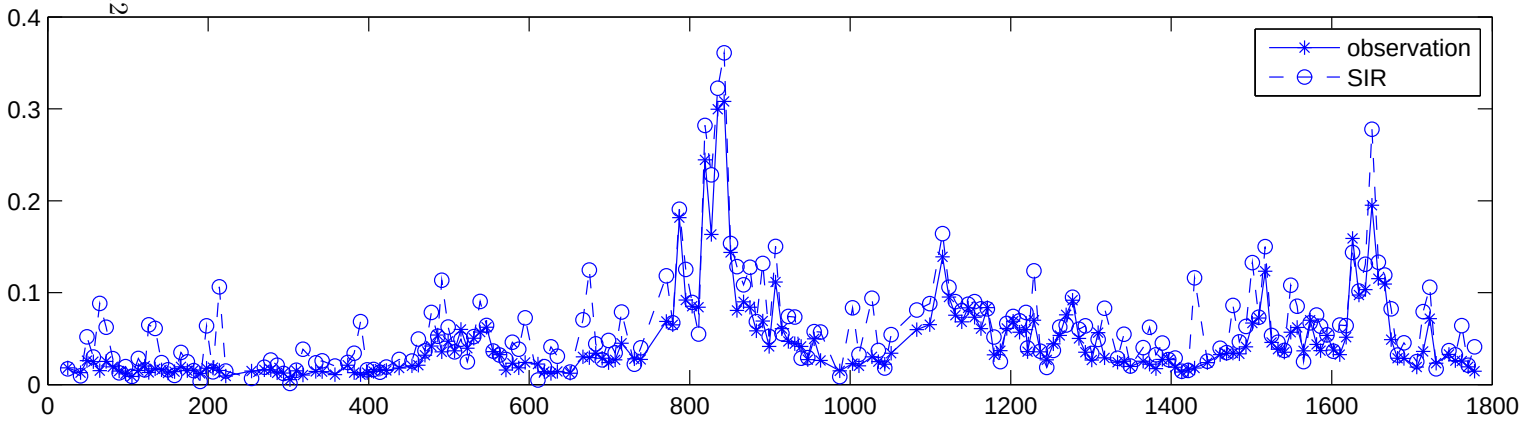
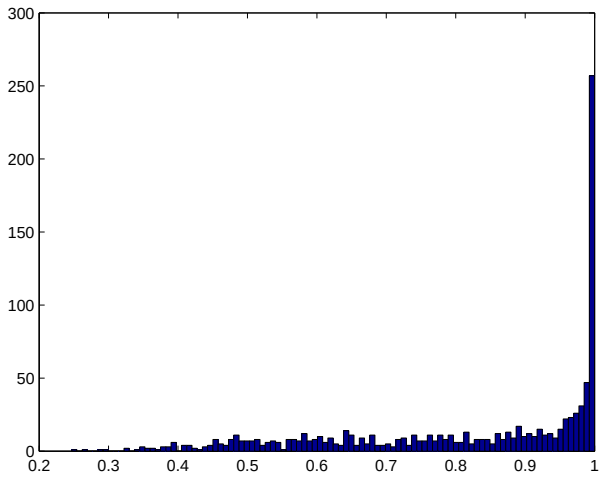


Figure 3: Results with $\sigma_P^2 = P(0)^2$ and 10 particles

Figure 4: Histogram of the SIR normalized maximum particle weights with 1000 runs for 100 dimensions



linear so that other effective ways of sampling it do exist. High-dimensional nonlinear problems where our filter may be indispensable will be presented elsewhere, in the context of specific applications.

8 Acknowledgments

We would like to thank Prof. J. Goodman, who urged us to write a more general version of our previous work and suggested some notations and nomenclature, Prof. R. Miller, who suggested that we try Dowd's model plankton problem as a first step toward an ambitious joint effort and helped us set it up, and Prof. M. Dowd, who kindly made the data available. This work was supported in part by the Director, Office of Science, Computational and Technology Research, U.S. Department of Energy under Contract No. DE-AC02-05CH11231, and by the National Science Foundation under grant DMS-0705910.

References

[1] M. Arulampalam, S. Maskell, N. Gordon, and T. Clapp. A tutorial on particle filters for online nonlinear/nongaussian Bayesia tracking. *IEEE Trans. Sig. Proc.*, 50:174–188, 2002.

[2] P. Bickel, B. Li, and T. Bengtsson. Sharp failure rates for the bootstrap particle filter in high dimensions. *IMS Collections: Pushing the Limits of Contemporary Statistics: Contributions in Honor of Jayanta K. Ghosh*, 3:318–329, 2008.

[3] S. Bozic. *Digital and Kalman Filtering.* Butterworth-Heinemann, Oxford, 1994.

[4] A. J. Chorin. Monte Carlo without chains. *Comm. Appl. Math. Comp. Sc.*, 3:77–93, 2008.

[5] A.J. Chorin and P. Krause. Dimensional reduction for a Bayesian filter. *Proc. Nat. Acad. Sci. USA*, 101:15013–15017, 2004.

[6] A.J. Chorin and X. Tu. Implicit sampling for particle filters. *Proc. Nat. Acad. Sc. USA*, 2009. to appear.

[7] A. Doucet, N. de Freitas, and N. Gordon. *Sequential Monte Carlo Methods in Practice*. Springer, New York, 2001.

[8] A. Doucet, S. Godsill, and C. Andrieu. On sequential Monte Carlo sampling methods for Bayesian filtering. *Stat. Comp.*, 10:197–208, 2000.

[9] A. Doucet and A. Johansen. Particle filtering and smoothing: Fifteen years later. *Handbook of Nonlinear Filtering (eds. D. Crisan et B. Rozovsky)*, to appear.

[10] M. Dowd. A sequential Monte Carlo approach for marine ecological prediction. *Environmetrics*, 17:435–455, 2006.

[11] W. Gilks and C. Berzuini. Following a moving target -Monte Carlo inference for dynamic Bayesian models. *J. Roy. Statist. Soc. B*, 63:127–146, 2001.

[12] J. Liu and C. Sabatti. Generalized Gibbs sampler and multigrid Monte Carlo for Bayesian computation. *Biometrika*, 87:353–369, 2000.

[13] S. Maceachern, M. Clyde, and J. Liu. Sequential importance sampling for nonparametric Bayes models: the next generation. *Can. J. Stat.*, 27:251–267, 1999.

[14] C. Snyder, T. Bengtsson, P. Bickel, and J. Anderson. Obstacles to high-dimensional particle filtering. *Mon. Wea. Rev.*, 136:4629–4640, 2008.

[15] J. Weare. Efficient Monte Carlo sampling by parallel marginalization. *Proc. Nat. Acad. Sc. USA*, 104:12657–12662, 2007.